List of subjects for the State (Leaving) Exam Study Programme: Chemistry and Technology Specialization: Chemistry

1. The course of the bachelor's state exam and the defence of the bachelor's thesis at the Faculty of Chemical Engineering is regulated according to the current version of the "Study and Examination Rules of the University of Chemistry and Technology (UCT) in Prague"

2. The state exam (SE) of the bachelor's programme has two parts, (i) the defence of the bachelor's thesis and (ii) the oral part of the SE, both taking place at the same day.

3. During the oral part of the SE a student has to answer questions related to **four** thematic areas. The list of the thematic areas for the SE assigned to this bachelor's programme is included below. All of the students have to take exam from the 1st and 2nd thematic area, all of the students have to select two of the 3rd-8th thematic areas from which they will be examined.

1. **General and Inorganic Chemistry** (based on the subjects AB101001 General and Inorganic Chemistry I and AN101002 General and Inorganic Chemistry II)

2. Organic Chemistry (based on the subjects AB110003 Organic Chemistry I and AB110004 Organic Chemistry II)

3. **Mathematics** (based on the subjects AB413001 Mathematics A, AB413002 Mathematics B, AB413003 Applied Statistics)

4. Physics (based on the subjects AB444003 Physics I, AB444004 Physics II)

5. Physical chemistry (based on the subjects AB403003 Physical Chemistry I, AB403004 Physical Chemistry II)

6. Biochemistry (based on the subjects AB32001 Biochemistry I, AB320005 Laboratory of Biochemistry)

7. Chemical Engineering (based on the subject AB409001 Unit Operations of Chemical Engineering I)

8. **Analytical Chemistry** (based on the subjects AB402001 Analytical Chemistry I and AB402002 Analytical Chemistry II)

The course of the State Exam usually proceeds as follows:

1. A staff member introduces the student to the members of the SE Committee.

2. The student will give a slideshow presentation of the main points of his/her thesis. (In exceptional cases, if a student will obtain approval from the chairman of the SE committee beforehand of the SE, he/she can use other forms of presentation.) The presentation should last 10 minutes at max. The following topics should be addressed in the presentation:

- the objectives of the thesis;
- a short description of the applied methodology;
- the specification of most important obtained results, their critical analysis;
- the conclusion and statement whether the thesis' objectives were fulfilled.

3. The thesis' review written by the supervisor is read.

4. The student answers questions and comments on points raised in the review of the reviewer. The student also answers questions from the members of the SE committee related to the topic of his/her thesis.

5. Oral examination. The student answers questions related to three thematic areas of the SE. (Duration about 30 minutes.)

6. The assessment of the student's performance in a closed (non-public) discussion of the SE committee.

7. The SE result announcement.

1. General and Inorganic Chemistry (based on the subjects AB101001 General and Inorganic Chemistry I and AN101002 General and Inorganic Chemistry II)

- 1. Atomic structure, electronic structure of atoms, atomic orbitals; periodic system, effective charge of atomic nuclei and its influence on periodic trends in physical-chemical properties of elements.
- 2. Chemical bonding bond types, energy character of inter- and intramolecular bonds; physical properties predictable using type of bonding.
- 3. Molecular Orbitals Theory bonding in diatomic molecules, bond order, and magnetism of molecules.
- 4. Valence Bond Theory; hybridization, Lewis structures, VSEPR; physical properties of molecules, molecular symmetry.
- 5. Lewis acid-base theory and its implications in inorganic chemistry; mechanisms of LA/LB reactions.
- 6. Acid-base theory; acid-base reactivity, simple ions and oxoanions in aqueous solutions, hydrolysis, solubility of salts; diagrams of predominant forms.
- 7. Coordination complexes; coordination bonding, ligand field splitting of d-orbitals; bonding types of ligands; structural isomerism and stereoisomerism.
- 8. Principles of redox reactions, reducing and oxidizing agents; standard reduction potentials; fundamentals of electrochemistry; Pourbaix diagrams.
- 9. Ionic bonding; structure and symmetry of crystalline solids; reactivity and properties of solid hydrides, halides, oxides, and other binary compounds of metals and p-elements.
- 10. Metallic bonding; trends in physical properties of metals; redox reactivity of metallic elements; production of important metals.

2. Organic Chemistry (based on the subjects AB110003 Organic Chemistry I and AB110004 Organic Chemistry II)

- 1. Alkanes and alkenes, radical and electrophilic addition, oxidation and reduction.
- 2. Alkynes and dienes, single and double electrophilic addition to alkynes, acidity of terminal alkynes, 1,2- and 1,4-addition to dienes, Diels-Alder reaction.
- 3. Arenes, electrophilic and nucleophilic substitution of arenes and heteroarenes, role of directing substituents, diazotization and reactions of diazonium salts, oxidation and reduction.
- 4. Haloalkanes bimolecular and monomolecular nucleophilic substitution and elimination.
- 5. Alcohols and phenols, bimolecular and monomolecular nucleophilic substitution, oxidation and reductions, transformation to alkyl alkan- and arensulfonates and their reactions.
- 6. Organometals, preparation and reactions; ethers including oxirane, preparation, applications and reactions.
- 7. Aldehydes and ketones, nucleophilic addition, oxidation and reduction.
- 8. Carboxylic acid and non-nitrogen functional derivatives of carboxylic acids acyl halides, anhydrides and esters, acylic (tetrahedral) nucleophilic substitution, reduction.
- 9. Reactions of enols and enolates, halogenation of aldehydes and ketones, aldol and Claisen condensation, acetoacetic and malonester synthesis.
- 10. Nitrogen containing compounds amines; nitrogen functional derivatives of carboxylic acid amides and nitriles and their reactions, acylic nucleophilic substitution of amides, reduction.
- 11. Heterocumulenes, α , β -unsaturated oxo compounds, carbonic acid derivatives.
- 12. Heterocycles, basic types of five- and six-membered heterocycles, aromaticity. Basicity, reactions on nitrogen, electrophilic and nucleophilic substitution reactions.
- 13. Amino acids and peptides, synthesis of coded amino acids, protection of terminal C- and N- groups of amino acids, peptide synthesis and analysis.
- 14. Saccharides, structure, stereochemistry, configuration, cyclic forms, oxidation and reduction, glycosides, reducing and non-reducing disaccharides, polysaccharides). Structure of nucleic acids, principles of base pairing.

3. Mathematics (based on the subjects AB413001 Mathematics A, AB413002 Mathematics B, AB413003 Applied Statistics)

- 1. Definition of derivative. Meaning in geometry and physics. Partial derivative and its geometric interpretation, gradient of a function. Partial derivative of composed function. Directional derivative.
- 2. Newton's and Riemann's definition of integral. Geometric a physical applications of definite integral. Mean value theorem for definite integrals.
- 3. First order differential equations, basic concepts. The method of separation of variables. First order linear differential equations, variation of constant.
- 4. Second order linear differential equation with constant coefficients and special form of right-hand side. The method of undetermined coefficients. Systems of two ordinary differential equations. Predator-prey model.
- 5. Matrices, matrix algebra. Linear dependence and independence of a group of vectors. Matrix rank. Systems of linear algebraic equations.
- 6. Determinant of matrix and its relationship to the matrix rank. Inverse matrix existence and calculation methods.
- 7. Function of two variables and its graph, contour lines of a graph. Local extrema of a function of two variables and their determination, stationary and saddle points.
- 8. Implicit functions, their existence a derivative.
- 9. Curves in plane and space, tangent vector. Vector field. Curve integral of a vector field and its independence of the path. Potential of a vector field.
- 10. Double integral and its geometric interpretation. Fubini's theorem and change of variables for double integrals. The Gaussian integral.
- 11. Numerical methods for initial and boundary value problems with ordinary differential equations.
- 12. Numerical methods for partial differential equations of parabolic type.

4. Physics (based on the subjects AB444003 Physics I, AB444004 Physics II)

- 1. Basic concepts of Mechanics I: Force, the Newton's laws, work, power, kinetic and potential energy. Conservation of mechanical energy and linear momentum, elastic and inelastic collisions.
- 2. Basic concepts of Mechanics II: Moment of inertia, torque, angular momentum. Work, power and energy in rotational motion. Conservation of mechanical energy and angular momentum.
- 3. Fluid mechanics: Hydrostatic pressure, Archimedes' law. Bernoulli's equation, real liquid flow.
- 4. Oscillations: undamped, damped and forced harmonic oscillations.
- 5. Waves: Description, propagation velocity, intensity. Huygen's principle, refraction and reflection, Snell's law.
- 6. Wave optics: Concept of light, interference, thin film, sigle-slit diffraction, diffraction grating.
- 7. Geometric optics: Basic concepts, reflection and refraction, optical instruments: magnifying glass, microscope.
- 8. Maxwell's equations.
- 9. Electromagnetic waves: Traveling, intenzity, energy transport, polarization, optical activity.
- 10. Inertial and non-inertial frames of reference, relativistic dynamics, the principle of equivalence.
- 11. Photons and the wave nature of particles: Compton effect, particle-wave duality, de Broglie wavelength, the uncertainty principle.
- 12. Schrödinger equation, particle in infinite potential well, energy level diagram.
- 13. The hydrogen atom, Bohr theory, energy level diagram, series of spectral lines.
- 14. Solid state physics: Band model, Fermi energy, intrinsic and doped semiconductor, PN transition.
- 15. Nuclear physics: Properties of nuclei, radioactivity, nuclear reactions. Elementary particles: fermions and bosons, quarks and leptons, forces.

5. Physical chemistry (based on the subjects AB403003 Physical Chemistry I, AB403004 Physical Chemistry II)

- 1. State behaviour of fluids. The equation of ideal gas, the van der Waals equation, virial equations of state. Critical point and critical properties of pure substances.
- 2. The first law of thermodynamics. Internal energy, enthalpy, work, heat, adiabatic processes.
- 3. The second and third laws of thermodynamics. Entropy, Gibbs and Helmholtz energies. Temperature and pressure dependences of basic thermodynamic functions.
- 4. Thermochemistry. Heat capacities, reaction heat, the Hess' and Kirchhoff's laws. Adiabatic temperature of reaction.
- 5. Thermodynamic description of mixtures. Partial molar quantities, excess and mixing quantities, chemical potential.
- 6. Activity and its standard states. Activity coefficients. Models for activity coefficients. Debye-Hückel theory and the mean activity coefficient.
- 7. The Gibbs's phase rule. Phase equilibrium of one-component systems. Clapeyron equation, Clausius-Clapeyron equation, phase diagrams.
- 8. Vapour-liquid and gas-liquid phase equilibria. The Raoult's and Henry's laws, typical phase diagrams, azeotropes.
- 9. Liquid-liquid and solid-liquid equilibria. Typical phase diagrams, thermodynamic description of equilibria in two-component systems. The lever rule.
- 10. Chemical and ionic equilibria. Equilibrium constant, mass balance, the response of equilibrium to the conditions.
- 11. Electrochemical processes. Electrolytic cells, the Faraday's law, galvanic cells, the Nernst equation, standard potentials.
- 12. Chemical kinetics of simple reactions. Rate laws, reaction order, rate constant and its temperature dependence, half-life of a reaction, integrated rate laws for reactions of zero, first, and second order. Chemical kinetics of simultaneous reactions.
- 13. Diffusion, migration of ions in electric field, conductivity, Kohlrausch law.
- 14. Surface chemistry. Interfacial tension, Laplace-Young and Kelvin equations. Adsorption.
- 6. Biochemistry (based on the subjects AB32001 Biochemistry I, AB320005 Laboratory of Biochemistry)
- 1. Amino acids and peptides. Protein structure and function.
- 2. Enzymes: common characteristic and classification. Enzyme kinetics.
- 3. Structure and function of nucleic acids, organization of prokaryotic and eukaryotic genome.
- 4. Replication: initiation, replication fork, recombination. Mutations and repair mechanisms.
- 5. Transcription, RNA polymerases, posttranscriptional modifications of RNA, splicing
- 6. mechanisms.
- 7. Basic concept of metabolism and energy conversion. Electron transport systems, citric acid cycle.
- 8. Metabolism of carbohydrates. Photosynthesis.
- 9. Metabolism of lipids.
- 10. Metabolism of nitrogen compounds.
- 11. Regulation of metabolic pathways.

7. Chemical Engineering (based on the subject AB409001 Unit Operations of Chemical Engineering I)

- 1. Material balances: intensive and extensive quantities, system and its boundaries, time (period) of balancing, stream, accumulation, source/sink (generation/consumption), fictitious streams, formulation of material balances, input matrix.
- 2. Fluid flow: laminar and turbulent flow, Reynolds number, continuity equation, Bernoulli equation, transport of fluids in pipes without/with a pump.
- 3. Cake filtration: mass balance of filtration, filtration rate, filtration equation, washing of the cake, type of filters.
- 4. Mixing: design rules for a mixing vessel, Power number for mixing, Reynolds number of mixing, Power correlations.
- 5. Mechanisms of heat transfer: convection, conduction, heat transfer in heat exchangers, calculation of heat transfer area.
- 6. Drying: mass and enthalpy balance of continuous dryers and a preheater (calorifer), mass balance of a batch dryer, calculation of drying time in a batch dryer.
- 7. Extraction mutually immiscible solvents: graphical solution of repeated (cross-flow) and counter-current extraction, equilibrium (theoretical) stage.
- 8. Distillation: principle of batch and flash distillation, schematics of counter-current distillation with reflux (rectification), material and enthalpy balances.
- 9. Chemical reactors: material balances of a batch reactor with ideal mixing, continuously stirred tank reactor with ideal mixing, and tubular reactor with plug flow.

8. Analytical Chemistry (based on the subjects AB402001 Analytical Chemistry I and AB402002 Analytical Chemistry II)

- 1. Basic terms (sample, analyte, matrix, interferent, analytical signal, analytical process, sampling methods, quartering). Characteristics of analytical methods trueness, accuracy, precision, limit of detection, limit of quantification, robustness, linear range, sensitivity.
- 2. Calibration methods (external calibration, standard addition, internal standard) and standards (chemical standard, reference material, certified reference material). Definitions of validation of analytical method and uncertainty of analytical measurement.
- 3. Volumetric analysis (basic concepts and principles of acid-base, precipitation, complexometric, and redox titration; titration curve, indication of the end of titration).
- 4. Gravimetric analysis (basic concepts and principles).
- 5. Electroanalysis (basic concepts and principles electrode types, selectivity, calibration)
- 6. Potentiometry and pH measurement (electrodes, direct potentiometry, potentiometric titration). Conductometry.
- 7. Voltammetry, polarography, and amperometry.
- 8. Coulometry, electrogravimetry.
- 9. Separation by chromatography and electro migration (overview and principles of particular techniques, important parameters and quantities, detection methods, qualitative and quantitative analysis).
- 10. Gas chromatography (overview and principles of particular techniques (adsorption and partition), detection methods, qualitative and quantitative analysis). Gas chromatography with mass spectrometry (interface, regime of MS spectra recording).
- 11. Liquid chromatography (overview and principles of particular techniques (normal, reverse-phase, sizeexclusion, ion exchange, chiral), detection methods, qualitative and quantitative analysis). Liquid chromatography with mass spectrometry (interface, regime of MS spectra recording).
- 12. Spectroscopy for chemical analysis (basic concepts and principles (absorption, emission, fluorescence, scattering). Calibration. Lambert-Beer's law and its use (quantities, deviations from validity, application).
- 13. Spectrometric instrumentation (basic building blocks of emission, absorption and fluorescence spectrometers).
- 14. Atomic spectrometry (overview and principles of individual techniques).
- 15. Molecular spectrometry (overview and principles of individual techniques).
- 16. Structure analysis (basic principles of IR, 1H and 13C-NMR, and mass spectra interpretation).
- 17. Mass spectrometry (instrumentation (building blocks of mass spectrometer), basic principles of ionization and ion separation techniques, application in qualitative and quantitative analysis). Mass spectrometry in hyphenated techniques.
- 18. Surface analysis (basic principles and applications of X-ray and ultraviolet photoelectron spectroscopy, Auger electron spectroscopy, and secondary ion mass spectrometry)
- 19. Bioanalytical chemistry (basic concepts and principles of enzymatic methods and immunoanalysis)
- 20. Radioanalysis (basic definitions (radioisotope, alpha, beta, gamma decay, activity, half-life time) and principles of gamma spectroscopy and neutron activation analysis)